

Phenol, 4-(1,1,4,4-tetramethylpentyl)

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|-----------------------------|------------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C15H24O/c1-14(2,3)10-11-15(4,5)12-6-8-13(16)9-7-12/h6-9,16H,10-11H2,1-5H1 |
| InchiKey: | IUGLBFMBSSODHQ-UHFFFAOYSA-N |
| Formula: | C15H24O |
| SMILES: | CC(C)(C)CCC(C)(C)c1ccc(O)cc1 |
| Mol. weight [g/mol]: | 220.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 38.89 | kJ/mol | Joback Method |
| hf | -311.21 | kJ/mol | Joback Method |
| hfus | 19.60 | kJ/mol | Joback Method |
| hvap | 61.68 | kJ/mol | Joback Method |
| log10ws | -4.18 | | Crippen Method |
| logp | 4.496 | | Crippen Method |
| mcvol | 204.320 | ml/mol | McGowan Method |
| pc | 2183.60 | kPa | Joback Method |
| rinpol | 1647.00 | | NIST Webbook |
| rinpol | 1658.00 | | NIST Webbook |
| rinpol | 1646.00 | | NIST Webbook |
| tb | 643.44 | K | Joback Method |
| tc | 868.39 | K | Joback Method |
| tf | 401.79 | K | Joback Method |
| vc | 0.712 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 563.32 | J/molxK | 643.44 | Joback Method |
| cpg | 581.66 | J/molxK | 680.93 | Joback Method |
| cpg | 598.70 | J/molxK | 718.42 | Joback Method |
| cpg | 614.58 | J/molxK | 755.91 | Joback Method |
| cpg | 629.45 | J/molxK | 793.40 | Joback Method |
| cpg | 643.47 | J/molxK | 830.89 | Joback Method |
| cpg | 656.77 | J/molxK | 868.39 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0012794 | Paxs | 401.79 | Joback Method |
| dvisc | 0.0004357 | Paxs | 442.07 | Joback Method |
| dvisc | 0.0001777 | Paxs | 482.34 | Joback Method |
| dvisc | 0.0000832 | Paxs | 522.62 | Joback Method |
| dvisc | 0.0000434 | Paxs | 562.89 | Joback Method |
| dvisc | 0.0000247 | Paxs | 603.17 | Joback Method |
| dvisc | 0.0000151 | Paxs | 643.44 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R591943&Units=SI |

Legend

| | |
|-----------------|-------------------------------------------------|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/54-930-9/Phenol-4-1-1-4-4-tetramethylpentyl.pdf>

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